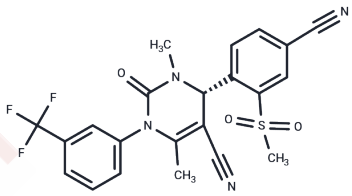
Data Sheet (Cat.No.T12613L)

TargetMol

BAY-85-8501

Chemical Properties



CAS No. : 1161921-82-9

Formula: C22H17F3N4O3S

Molecular Weight: 474.46

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	BAY-85-8501 is a selective, reversible, and potent inhibitor of Human Neutrophil Elastase (HNE) with an IC50 of 65 pM.
Targets(IC50)	Serine Protease
In vivo	In this study, the exogenous compound HNE noxa is identified as the primary cause of lung injury and hemorrhage. BAY-85-8501 (29), due to its picomolar potency against HNE and high effectiveness against MNE, completely prevents lung injury and subsequent inflammation if administered one hour before exposure to HNE noxa. Despite its high selectivity for HNE inhibition, BAY-85-8501 does not prevent primary lung injury caused by PPE since it has no effect on it. However, BAY-85-8501 can inhibit MNE, an endogenous promoter of inflammation and secondary lung injury, albeit with lower potency. The prevention of inflammation and secondary injury by BAY-85-8501 is less pronounced and requires doses 30 times higher than standard. Its effectiveness primarily relies on its ability to inhibit MNE (Ki=6 nM) in these cases. At a dosage of 0.01 mg/kg, a significant reduction in hemoglobin concentration is noted, and at 0.1 mg/kg, a notable decrease in neutrophil count is observed, indicating efficacy is largely dependent on its potency against HNE (Ki=0.08 nM) in this scenario.

Solubility Information

Solubility	DMSO: 200 mg/mL (421.53 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 5 mg/mL (10.54 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.1077 mL	10.5383 mL	21.0766 mL
5 mM	0.4215 mL	2.1077 mL	4.2153 mL
10 mM	0.2108 mL	1.0538 mL	2.1077 mL
50 mM	0.0422 mL	0.2108 mL	0.4215 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Von Nussbaum F, et al. Freezing the Bioactive Conformation to Boost Potency: The Identification of BAY 85-8501, a Selective and Potent Inhibitor of Human Neutrophil Elastase for Pulmonary Diseases. ChemMedChem. 2015 Jul;10 (7):1163-73.